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Multi-objective synthesis of work and heat exchange networks: Optimal balance between economic and environmental performance.

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ABSTRACT

Sustainable and efficient energy use is crucial for lessening carbon dioxide emissions in industrial plants. This paper introduces a new bi-criteria optimization model for the environmentally conscious synthesis of work and heat exchange networks (WHEN),

focused on enhancing their environmental and economic performance. Thus, the proposed multistage superstructure allows power and thermal integration of process gaseous streams, by the simultaneous minimization of environmental impacts and total annualized cost. We present a set of alternative Pareto solutions to support decision-makers towards the implementation of more environment-friendly and cost-effective WHEN networks.

Keywords: Multi-objective optimization (MOO), work and heat exchange networks (WHEN), life cycle assessment (LCA), cost analysis.

1. Introduction

Environmental impact caused by increasing gaseous emissions and the rapid depletion of fossil fuels reserves is a major global concern. Due to the rising interest in the development of more sustainable and efficient energy processes, multi-objective optimization (MOO) has arisen as a useful design and planning tool [1–4]. In fact, MOO is able to simultaneously deal with conflicting environmental and economic goals, allowing to identify the best alternatives balancing the bi-criteria problem [5,6].

Pressure manipulation is an energy-intensive process particularly important in synthetic methanol and ammonia synthesis, oil refineries and cryogenic production of liquefied natural gas (LNG). In such plants, the integration between work and heat can be very interesting for achieving significant savings in energy and processing costs [7–12]. The recognized importance of heat integration, and more recently, power integration, in process synthesis is stressed by the increasing literature about these aspects during the last few years. An important contribution to this area is addressed to

Huang and Fan [13]. In their work, the authors have introduced first insights about work exchange networks (WENs), defining the main operational principles for the process.

In Aspelund et al. [14], a heuristic graphical-based approach is used for energy requirements minimization in heat exchanger networks (HENs) considering pressure levels adjustment of process streams at sub-ambient conditions. Grounded on the previous work (ref. [14]), Wechsung et al. [15] have developed a model for HENs synthesis with integrated pressure manipulation, combining mathematical programming, pinch and exergy analyses. The authors have successfully applied the model to LNG production, showing that process total irreversibility can be decreased through a specific compression and expansion route of streams.

Afterwards, Onishi et al. [9] have employed this pressure manipulation route to formulate a superstructure for simultaneous HENs synthesis, aiming to enhance heat integration by power recovery. The mathematical model is formulated using generalized disjunctive programming (GDP), and optimized via mixed-integer nonlinear programming (MINLP) by minimizing the total annualized cost. The authors have demonstrated that optimal integration between work and heat significantly improves the process energy efficiency, reducing capital and operational costs related to the LNG process. The model has been posteriorly extended by Onishi et al [11] for the retrofit of existing HENs.

Razib et al. [7] have proposed an optimization model for preliminary WEN synthesis. In their work, the problem is formulated using mathematical programming techniques with the objective of minimizing the total annual cost. However, these authors have not considered heat integration of process streams. To address this issue, Onishi et al. [10] have developed a MINLP model for WENs optimization, allowing streams thermal integration. Their results emphasize that simultaneous heat integration between pressure manipulation stages is crucial for improving the WEN cost-effectiveness. Fu and Gundersen [16] have studied the correct placement of pressure manipulation equipment coupled to HENs at above ambient conditions. A graphical approach is developed for HENs design containing compressors and expanders, for minimization of exergy consumption. In 2016, Fu and Gundersen [17] have proposed new thermodynamic insights based on pinch analysis for the application of work and heat integration to CO_2 capture processes. The authors have shown that optimal integration between work and heat can lead to considerable energy savings in oxy-combustion and post-combustion membrane-based separation processes.

Although the above-mentioned works can represent important contributions for the process systems engineering (PSE) field, none of them has considered environmental concerns during the network design task. To surpass this limitation, we introduce a new bi-criteria model for the environmentally conscious synthesis of work and heat exchange networks (WHENs). To the best of our knowledge, this is the first study to carry out the WHEN design through the simultaneous optimization of its environmental and economic performance. Hence, the main novelty of this work relies in the assessment of the environmental impacts associated to energy services consumption in WHEN synthesis. The life cycle assessment (LCA)-based Eco-indicator 99 is used to evaluate the environmental criteria. The proposed model is formulated via multi-objective mixed-integer nonlinear programming (moMINLP), and solved by the standard ε-constraint method. A case study is performed to obtain a set of optimal alternative Pareto solutions. The Pareto curve can be used to support decision-makers for implementing more sustainable and economical work and heat integration processes.

2. Problem statement

Given is a set of process gaseous streams at low-pressure (LP) and high-pressure (HP), in addition to equipment for pressure and heat exchange, as well as electric power and thermal utilities (including cooling water and steam), and their corresponding costs. The LP streams need to be compressed from a known supply state (defined by their inlet temperatures and pressures, mass flowrates and specific heat) to their target temperatures and higher pressures. Analogously, the HP streams need to be expanded from a determinate supply condition (stated by their inlet temperatures and pressures, mass flowrates and specific heat) to their target temperatures and lower pressures. Furthermore, environmental impacts accounted during the entire life cycle by the Eco-indicator 99 methodology for each energy service (*i.e.*, cooling water, steam and electricity) are also available. In this paper, we address the problem of obtaining the optimal WHEN configuration that simultaneously minimizes the overall environmental impact and total annualized cost of the process.

3. Multi-objective WHEN synthesis

The multi-objective WHEN synthesis is a very difficult task aimed at designing synchronously both WEN and HEN, by the minimization of two different objective functions at once. Regarding the WEN design, power integration of process gaseous streams is carried out through a multistage superstructure as developed by Onishi et al. [10]. Thus, LP and HP streams should exchange work via stand-alone pressure manipulation equipment, and turbines and compressors running on common single-shaft-turbine-compressor (SSTC). Between each WEN compression and expansion stage, LP and HP streams are conducted towards the HEN to enhance pressure recovery by promoting heat integration. Moreover, helper motors and generators are placed on the SSTC axis units to fill for power shortages and to convert energy excesses into electricity, respectively. A more detailed description of the WEN process can be found in Onishi et al. [10]. On the other hand, the HEN synthesis is based on the well-known deterministic superstructure proposed by Yee and Grossmann [18], in which stream splits are allowed and constant heat transfer coefficients and isothermal mixing are assumed, for simplifying the model.

It is worth to mention that, as compression efficiency is favored by lower inlet temperatures and expansion efficiency is better at higher inlet temperatures, LP streams are considered as hot streams, while HP streams are treated as cold streams for heat integration. **Fig. 1** displays the multistage WHEN superstructure with the main decision variables considered for multi-objective optimization. Note that all inlet and outlet temperatures and pressures in the WHEN superstructure are unknown optimization variables. For this reason, both temperatures and pressures play a critical role during the WHEN synthesis. In addition, the high nonlinearity and non-convexity of the mathematical formulation for pressure equipment design, temperature approximation and cost estimation further increase the WHEN model complexity and, consequently, the difficult to solve it in a reasonable CPU time.

The damage-oriented Eco-indicator 99 [19–21] methodology based on the LCA principles is used to evaluate the environmental criteria. Thus, the environmental objective function accounts for the overall impacts obtained from Eco-indicator 99 method for all thermal services and electricity consumed in the process. By contrast, the economic objective function corresponds to the minimization of the process total annualized cost. The contributions of operational expenses related to electricity and thermal utilities consumption, and capital cost of investment in all equipment that compose the WHEN are considered in the objective function. The mathematical model for the multi-objective WHEN synthesis is presented in the following sections.

4. Mathematical model for the sustainable WHEN synthesis

The mathematical formulation is based on our previous study presented in Onishi et al. [10], in which a simultaneous model for the optimal WEN synthesis have been proposed considering heat recovery of process streams. Therefore, the WHEN optimization model is composed by equipment design equations (including compressors, turbines, valves, heat exchangers, heaters and coolers), energy and mass balances in all pressure manipulation and heat exchange stages, logical constraints, temperature and pressure feasibility restrictions, and objective functions. The mathematical formulation for the WEN design is presented in **Appendix A**.

The goal of the proposed mathematical model is to optimize the WHEN synthesis, taking into account the environmental impact and economic performance of the process. The problem is mathematically formulated as a moMINLP model and implemented in GAMS software (version 24.6.1). The minimization of two distinct objective functions is considered for optimizing the problem. The environmental and economic objective functions, as well as the solution procedure are described as follows.

4.1 Environmental objective function

As aforementioned, the environmental impact of the WHEN is evaluated through the LCA-based Eco-indicator 99. Note that the LCA methodology allows quantifying the overall environmental damage caused by an activity, product and/or process throughout their entire life cycle [20,22]. Three major impact categories are considered in the Eco-indicator 99 methodology: (*I*) damage to human health; (*II*) damage to ecosystem quality; and, (*III*) damage to resources. These impact categories are divided in eleven damage subcategories, including climate change, ionizing radiations and ozone layer depletion effects on human health; gaseous emissions, land occupation, acidification and eutrophication effects on ecosystem quality; and, minerals and fossil fuels extraction effects on the resources, to mention a few. The Eco-indicator 99 is estimated by the following equation.

$$Ecoindicator = \sum_{ic} \sum_{de \in D(ic)} \theta_{ic} \cdot \varpi_{ic} \cdot \delta_{de} \qquad (1)$$

In which,

$$\delta_d = \sum_{de} \alpha_{de} \cdot \beta_{de_d} \qquad (2)$$

In **Eq. (1)**, δ represents the damage category, while θ and ϖ are normalization and weighting factors, respectively. In **Eq. (2)**, α_{de} is a parameter associated to the direct releases, raw materials production and energy generation, and β_{de} is the damage factor related with each impact category ic. Note that the Hierarchist perspective is considered for the LCA approach [19]. In this work, we consider a "*cradle-to-gate*" analysis comprising all life cycle stages of the thermal utilities and electricity consumed in the WHEN. Therefore, the Eco-indicator 99 estimated for each energy service considers the environment impacts caused by the resources and raw materials extractions, fossil fuels consumption and pollutants emissions.

The environmental objective function is expressed by the product between the consumed electricity amount (by stand-alone compressors and helper motor) and the power electric Eco-indicator 99; plus, the products between consumed heating and cooling services and their corresponding Eco-indicators 99. The resulting objective function is annualized by the parameter f_{EI} as follows:

$$\min \quad EI = f_{EI} \left[\begin{array}{l} Ecoindicator_{electricity} \cdot \left(\sum_{i=1}^{LP} \sum_{s=1}^{S} Wc_{i,s} + \sum_{e=1}^{E} Whm_{e} \right) \\ + \sum_{m=1}^{M} \sum_{j=1}^{J} Ecoindicator_{steam} \cdot Q_{m,j} + \sum_{i=1}^{I} \sum_{n=1}^{N} Ecoindicator_{cooling\_water} \cdot Q_{i,n} \end{array} \right] \quad (3)$$

4.2 Economic objective function

The economic performance of the WHEN network is assessed by the minimization of the objective function composed by the total annualized cost (TAC). The process total cost comprises the contributions related to operational expenses ($OPEX$), and capital cost of investment in equipment ($CAPEX$). In this way, the operational expenses are associated to electricity and thermal services consumption (cooling and heating fluids), while capital cost consists of the expenditure in all units that compose the WHEN (*i.e.*, stand-alone and SSTC compressors, stand-alone and SSTC turbines, valves, helper motors, electric generators, heat exchangers, heaters and coolers). The economic objective function is expressed by **Eq. (4)**.

$$\min \quad TAC = OPEX + CAPEX \quad (4)$$

In which,

$$OPEX = \left[\begin{array}{l} c_{elec} \cdot \left(\sum_{i=1}^{LP} \sum_{s=1}^{S} Wu_{i,s} + \sum_{e=1}^{E} Wm_{e} \right) - c_{elec\_sale} \cdot \left(\sum_{j=1}^{HP} \sum_{s=1}^{S} Wu_{j,s} + \sum_{e=1}^{E} Wg_{e} \right) \\ + c_{steam} \cdot \sum_{m=1}^{M} \sum_{j=1}^{J} Q_{m,j} + c_{cooling\_water} \cdot \sum_{h=1}^{H} \sum_{n=1}^{N} Q_{h,n} \end{array} \right] \tag{5}$$

$$CAPEX = fac \cdot \left(\frac{CEPCI^{2015}}{CEPCI^{2003}} \right) \cdot \left[\begin{array}{l} \left(\begin{array}{l} F_{BM}^{V} \cdot \sum_{j=1}^{HP} \sum_{s=1}^{S} C_{PO}^{V} \cdot y_{j,s}^{V} + F_{BM}^{TU} \cdot \sum_{j=1}^{HP} \sum_{s=1}^{S} C_{PO\,j,s}^{TU} + F_{BM}^{GE} \cdot \sum_{e=1}^{E} C_{PO\,e}^{GE} \\ F_{BM}^{CU} \cdot \sum_{i=1}^{LP} \sum_{s=1}^{S} C_{PO\,i,s}^{CU} + 1.2 \cdot F_{BM}^{TA} \cdot \sum_{j=1}^{HP} \sum_{s=1}^{S} \sum_{e=1}^{E} \sum_{k=1}^{K} C_{PO\,j,s,e,k}^{TA} \\ +1.2 \cdot F_{BM}^{CA} \cdot \sum_{i=1}^{LP} \sum_{s=1}^{S} \sum_{e=1}^{E} \sum_{k=1}^{K} C_{PO\,i,s,e,k}^{CA} + F_{BM}^{HM} \cdot \sum_{e=1}^{E} C_{PO\,e}^{HM} \end{array} \right) \\ + \left(\begin{array}{l} F_{BM}^{HE} \cdot \sum_{h=1}^{H} \sum_{c=1}^{C} \sum_{t=1}^{T} C_{PO\,h,c,t}^{HE} + F_{BM}^{Cooler} \cdot \sum_{h=1}^{H} \sum_{n=1}^{N} C_{PO\,h,n}^{HE} \\ + F_{BM}^{Heater} \cdot \sum_{m=1}^{M} \sum_{c=1}^{C} C_{PO\,m,c}^{HE} \end{array} \right) \end{array} \right] \tag{6}$$

In **Eq. (5)**, c_{elec}, c_{elec_sale}, c_{steam} and $c_{cooling\_water}$ are parameters for cost of power electric purchase, electricity sale, and heating and cooling services, respectively. In **Eq. (6)**, F_{BM} corresponds to the correction factor for the unitary cost that considers operational conditions and construction materials. C_{PO} is the unitary device cost (in US$) at operational pressure close to ambient conditions. In this work, C_{PO} is estimated using the cost correlations proposed by Couper [23] for pressure manipulation equipment (*i.e.*, turbines, compressors, electricity generators, helper motors and valves). Whereas the correlations presented by Turton et al. [24] are used for the unitary cost estimation of the thermal equipment, including heat exchangers, coolers and heaters. The cost correlations should be adjusted for the year of interest according the CEPCI index (Chemical Engineering Plant Cost Index). In addition, the parameter fac is the factor of annualized capital cost as defined by Smith [25]. Note that the pressure manipulation equipment running on common SSTC shafts are considered 20% more expensive than the same equipment out the shaft (*i.e.*, stand-alone equipment).

4.3 Solution procedure: ε-constraint method

The moMINLP problem as stated in this work can be expressed as follows:

$$\begin{aligned} &\min_{x,y} \quad EI(x),\ TAC(x,y) \qquad x \in \mathbb{R},\ y \subset \{0,1\} \\ &s.t. \quad \text{all design constraints} \end{aligned} \tag{7}$$

In which, EI denotes the environmental impact as defined by **Eq. (4)**, and TAC is the total annualized cost estimated by **Eq. (4) – Eq. (6)**. x and y represents the continuous and binary variables, respectively, which are associated to operational and designing decisions. The moMINLP model is subjected to all design equality and inequality constraints and solved using the ε-constraint method [26]. The ε-constraint method is based on the formulation of an auxiliary single-objective model, in which one of the goals is maintained as a main objective, while the other one is considered as a constraint. The single-objective problem is solved for distinct epsilon bound values imposed on the constraints. A different Pareto solution is generated for each considered epsilon bound. Therefore, the solution of the proposed moMINLP model is given by a set of Pareto alternatives, each one representing the optimal trade-off between the environmental and economic objectives. Note that from these set of points, the Pareto curve can be constructed allowing decision-makers to identify the best WHEN option to be considered for implementation.

5. Results and discussion

A case study is performed to verify the applicability of our proposed environmental conscious approach for the simultaneous multi-objective WHEN synthesis. In this example, we consider the work and heat integration between two high-pressure streams (HP1 and HP2) and two low-pressure streams (LP1 and LP2). Thus, the high-pressure streams HP1 and HP2 should be expanded from an inlet condition of 850 kPa (at 350 K) and 980 kPa (at 320 K) to a target condition of 100 kPa (at 350 K) and 180 kPa (at 320 K), respectively. On the other hand, the low-pressure streams LP1 and LP2 should be compressed from an inlet condition of 100 kPa (at 420 K and 450 K, correspondently) each one to a target state defined by 520 kPa (at 420 K) and 850 kPa (at 450 K), respectively. The stream data and environmental and cost parameters are shown in **Table 1**. Additional data includes heat transfer coefficients for all streams equal to 0.1 kW $(m^2\,K)^{-1}$, and for heating and cooling services equal to 1.0 kW $(m^2\,K)^{-1}$. Steam and cooling water are available at 483 K and 293 K, correspondingly. All unknown streams temperatures are limited between 298 and 600 K. A factor of 0.18 is considered for the annualization of capital cost of investment in equipment, corresponding to 10% of interest ratio over a period of 8 years of amortization. The environmental indicator is annualized by considering a factor of 8000 hr $year^{-1}$.

Single-objective problem: EI minimization

The solution of the single-objective problem without considering the economic objective function (*i.e.*, environmental impact minimization) is displayed in **Figure 2**. This solution corresponds to the green point in the Pareto curve as shown in **Figure 3**.

The optimal WHEN configuration found is comprised by seven turbines (1,052.47 kW; 679.49 kW; 630.44 kW; 584.94 kW; 533.54 kW; 701.96 kW; and, 631.46 kW, respectively) and eight compressors (688.88 kW; 836.98 kW; 950 kW; 90.6 kW; 950 kW; 283.55 kW; 950 kW; and, 453.33 kW, respectively) allocated on the SSTC axis, in addition to a valve and a stand-alone compressor (759.33 kW), which are used as pressure manipulation equipment. In this case, a single SSTC unit is needed in which the total expansion work is equal to 4,814.3 kW, while the total compressor work is equal to 5,203.36 kW. For this reason, a helper motor (389.06 kW) is still required at the SSTC to satisfy the energy balance on such axis. Furthermore, the WHEN is composed by five heat exchanges (1,481.81 kW – 3,757.72 m^2; 853.16 kW – 3,000 m^2; 983.82 kW – 2,763.11 m^2; 612.37 kW – 1,086.27 m^2; and, 883.48 kW – 2,857.90 m^2) and two coolers (448.21 kW – 449.46 m^2 and 669.84 kW – 870.16 m^2) utilized for energy integration in the network.

The total environmental impact of the optimal WHEN solution accounted by the Eco-indicator 99 is equal to 450,476. The correspondent total annualized cost of the WHEN is equal to 9,684 kUS\$ $year^{-1}$, involving 8,592 kUS\$ $year^{-1}$ associated to capital cost of investment in equipment and 1,092 kUS\$ $year^{-1}$ related to operational expenses (including thermal utilities with 115 kUS\$ $year^{-1}$, and electricity services with 977 kUS\$ $year^{-1}$).

Single-objective problem: TAC minimization

The solution of the single-objective problem without considering the environmental objective function (*i.e.*, total annualized cost minimization) is depicted in **Figure 4**. Note that this solution is related to the blue point alternative in the Pareto curve displayed in **Figure 3**.

In this case, the optimal WHEN configuration is composed by eight SSTC turbines (1,500 kW; 270.64 kW; 583.17 kW; 200 kW; 100 kW; 190.62 kW; 1,500 kW;

and, 40.12 kW, respectively) and five compressors (950 kW; 36 kW; 950 kW; 794.34 kW; and, 950 kW, respectively) placed on two different axis units. Moreover, the optimal WHEN needs a valve and three stand-alone compressors (388.59 kW; 950 kW; and, 950 kW, respectively) for recovering work in the network. Thus, the total expansion work in the first axis is equal to 2,615.91 kW, while the total compressor work consumed in such shaft is equal to 1,936 kW. In consequence, a generator of 679.91 kW of capacity should be used in the first SSTC unit to fulfill for the energy requirements on such axis. Analogously, the second shaft has the total expansion work equal to 1,770.64 kW, and 1,744.34 kW of total compressor work. For this reason, a generator of 26.3 kW of capacity should be placed on the second shaft unit. In addition, the WHEN is comprised by three heat exchanges (653.68 kW – 483.39 m^2; 2,000.13 kW – 1,384.93 m^2; and, 1,733.44 kW – 761.23 m^2) and two coolers (288.46 kW – 119.27 m^2 and 1,293.23 kW – 430.89 m^2) for allowing heat integration in the network.

The total annualized cost of the WHEN is equal to 7,404 kUS\$ $year^{-1}$, including 5,829 kUS\$ $year^{-1}$ related to capital cost of investment in equipment and 1,575 kUS\$ $year^{-1}$ associated to operational expenses (consisting of 158 kUS\$ $year^{-1}$ in cooling services and 1,417 kUS\$ $year^{-1}$ in electricity). In this case, the correspondent total environmental impact of the optimal WHEN solution accounted by the Eco-indicator 99 is equal to 897,317.

The first solution obtained for the EI minimization (*i.e.*, extreme solution represented by the green point in the Pareto curve in **Figure 3**) has a total compression work approximately 0.1% lower than the work generated in the WHEN with minimum cost (*i.e.*, extreme solution represented by the blue point in the Pareto curve in **Figure 3**). However, the WHEN with minimum EI presents the total expansion work ~8,9% higher than the solution found by the cost minimization. Moreover, the WHEN with minimum TAC needs a total heat transfer area ~78,5% smaller than the same equipment required in the network with minimum EI. Consequently, the solution found in the second case (blue point) represents a decreasing around ~32% in the capital cost of investment. Nevertheless, the WHEN obtained by the TAC minimization presents operational expenses ~44,2% greater than the network with minimum EI. Note that the difference in the TAC for both solutions is equal to ~23,5%, while the EI is increased in ~99,2% by minimizing the network costs. The optimal results obtained for both extreme solutions in the case study are shown in **Table 2**.

Multi-objective problem: set of Pareto optimal solutions

The Pareto curve displayed in **Figure 3** contains a set of optimal trade-off solutions that simultaneous balance the multi-objective problem. These solutions have been obtained by applying the ε-constraint method, by minimizing both TAC and EI objective functions. We emphasize that the extreme solutions (green and blue points represented in the Pareto curve) above presented can be impractical for many reasons, including the amount of equipment required in the network, capital and operational costs, and related environmental impacts. In consequence, the proposed approach is very interesting as it allows determining the best alternatives according to decision-maker's requirements.

Note that the first solutions of the Pareto curve (*i.e.*, solutions closer to the green point) are dominated by lower environmental impacts and, consequently, higher total annualized costs. This is because the capital costs related to heat and work exchanger equipment are typically more elevated in this region of the Pareto curve. By contrast, the last solutions of the Pareto frontier (*i.e.*, solutions nearer to the blue point) are dominated by lower TAC and, therefore, higher EI. In this region, the increased operational expenses and, obviously, higher EI associated to cooling and electricity services can make the WHEN configurations unviable. The best alternatives are represented by the intermediate region, in which both economic and environmental criteria can be considered in the network. Therefore, the main advantage of the developed model is its capability to obtain a set of optimal alternative trade-off solutions for WHEN design that allows to construct a Pareto curve. This set of Pareto solutions can be used by decision-makers for the implementation of more environment-friendly and cost-effective WHEN networks.

As mentioned before, we have written the developed WHEN model using GAMS, solving via DICOPT (under an increased major iterations number of 25) solver (with CONOPT and CPLEX as sub-solvers). In this work, we have used a personal computer with an Intel Core i5-2520M 2.5 GHz processor and 8 GB RAM running Windows 8.1. The CPU time did not exceed 10 min. It is worth to mention that lower and upper bounds applied for critical variables such as: streams mass flowrates; compression and expansion works; and, streams pressure and temperature are crucial for solving the problem in a reasonable time. The mathematical model for the multi-objective WHEN synthesis includes 3,427 continuous variables, 51 discrete variables and 4,827 equality and inequality constraints with 14,247 Jacobian elements (non-null), of which 2,046 are nonlinear.

6. Conclusion

In this work, we introduce a new multi-objective mathematical model for the environmentally conscious WHEN synthesis. To the best of our knowledge, this is the first study about the optimization of the WHEN design through simultaneous minimization of conflicting environmental and economic objective functions. To this aim, we propose a multistage superstructure allowing power and thermal integration of process gaseous streams, focused on enhancing the process environmental and economic performance. The proposed model is formulated via moMINLP, and solved by using the standard ε-constraint method.

The LCA-based Eco-indicator 99 methodology is applied to evaluate the environmental criteria. We consider the environmental impact caused by energy services consumed in the network including cooling and electricity services, throughout their entire life cycle. In contrast, the economic objective function corresponds to the minimization of the process total annualized cost. Thus, the contributions related to capital cost of investment in all WHEN equipment, as well as operational expenses associated to electricity and thermal utilities consumption are included in the objective function.

A case study is carried out to obtain a set of optimal alternative Pareto solutions. Results highlight the conflict existing between economic and environmental objectives during the WHEN synthesis. Thus, our proposed multi-objective approach can represent a very attractive and useful tool because it is suitable to determine the best alternatives according to process requirements that simultaneous balance both criteria. Therefore, our developed multi-objective model can be used to support decision-makers towards the implementation of more environment-friendly and cost-effective WHEN networks.

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Nomenclature

Roman letters

Cp	Heat capacity
C_{PO}	Unitary cost
CR_{max}	Maximum compression ratio
f_{ac}	Annualization factor for the capital cost
f_{EI}	Annualization factor for the environmental impact
EI	Environmental impact
F	Streams flowrate
Fb	Bypass flowrate
F_{BM}	Correction factor for capital cost
Fe	SSTC equipment flowrate
Fv	Valve flowrate
Fu	Stand-alone equipment flowrate
M	Big-M reformulation parameter
OPEX	Operational expenses
P	Streams pressure
P_{IN}	Network inlet pressure
Pin	Stage inlet pressure
P_{OUT}	Network outlet pressure
$Pout$	Stage outlet pressure
Q	Heat flow
T	Streams temperature
TAC	Total annualized cost
T_{IN}	Network inlet temperature

Tin	Stage inlet temperature
T_{OUT}	Network outlet temperature
Tout	Stage outlet temperature
Tturb	Outlet temperature of turbines
Tval	Outlet temperature of valves
We	Work of SSTC equipment
Wg	Work of generators
Wm	Work of helper motors
Wu	Work of utility equipment
y	Binary variable to define the existence of SSTC equipment
y^a	Binary variable auxiliary
y^B	Binary variable to define the existence of a bypass
y^U	Binary variable to define the existence of utility equipment
y^V	Binary variable to define the existence of valves

Acronyms

CEPCI	Chemical Engineering Plant Cost Index
GAMS	General Algebraic Modeling System
GDP	Generalized Disjunctive Programming
HEN	Heat Exchanger Network
HP	High-Pressure
LCA	Life Cycle Assessment
LNG	Liquefied Natural Gas
LP	Low-Pressure
MINLP	Mixed-Integer Nonlinear Programming
MOO	Multi-Objective Optimization

moMINLP	Multi-Objective Mixed-Integer Nonlinear Programming
SSTC	Single-Shaft-Turbine-Compressor
PSE	Process Systems Engineering
WEN	Work Exchange Network
WHEN	Work and Heat Exchange Network

Greek letters

α_{de}	Process burdens for energy utilities
β_{de}	Damage factor produced by each damage category
δ	Damage category
γ	Heat capacity ratio
η	Isentropic efficiency
μ	Joule-Thompson coefficient
ϖ	Weighting factor for the damage category
θ	Normalization factor

Subscripts

e	SSTC axes
i	LP streams
ic	Impact category
j	HP streams
k	Streams splits
m	Heating utility
n	Cooling utility
s	Stages in the WEN

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Fig. 1. Multistage superstructure with main decision variables considered for the multi-objective WHEN synthesis.

Fig. 2. Optimal WHEN configuration with minimum total environmental impact.

Fig. 3. Pareto curve of optimal alternative trade-off solutions for the case study.

Fig. 4. Optimal WHEN configuration with minimum total annualized cost.

Appendix A. Mathematical model for optimal WEN synthesis

The mathematical formulation for the optimization of WENs synthesis is presented in the following sections.

A.1 Sets definition

The next sets are required for the development of the model.

$$
\begin{gathered}
HP = \{ j \,/\, j = 1,2,...,HP \text{ indicates the high pressure streams}\} \\
LP = \{ i \,/\, i = 1,2,...,LP \text{ indicates the low pressure streams}\} \\
S = \{ s \,/\, s = 1,2,...,S \text{ indicates the network stages}\} \\
K = \{ k \,/\, k = 1,2,...,K \text{ indicates the stream splits}\} \\
E = \{ e \,/\, e = 1,2,....,E \text{ indicates the shaft units}\}
\end{gathered}
$$

A.2 Logical relationships

The following binary variables are used for the selection of the network equipment.

$$
\begin{aligned}
y_{i,s,e,k} &= \begin{cases} 1 & \text{if stream } i \text{ uses a compressor on unit } e, \text{ stage } s \text{ and split } k \\ 0 & \text{otherwise} \end{cases} && i \in LP, s \in S, e \in E, k \in K \\
y_{j,s,e,k} &= \begin{cases} 1 & \text{if stream } j \text{ uses a turbine on unit } e, \text{ stage } s \text{ and split } k \\ 0 & \text{otherwise} \end{cases} && j \in HP, s \in S, e \in E, k \in K \\
y^{U}_{i,s} &= \begin{cases} 1 & \text{if stream } i \text{ uses a stand-alone compressor in stage } s \\ 0 & \text{otherwise} \end{cases} && i \in LP, s \in S \\
y^{U}_{j,s} &= \begin{cases} 1 & \text{if stream } j \text{ uses a stand-alone turbine in stage } s \\ 0 & \text{otherwise} \end{cases} && j \in HP, s \in S \\
y^{V}_{j,s} &= \begin{cases} 1 & \text{if stream } j \text{ uses a valve in stage } s \\ 0 & \text{otherwise} \end{cases} && j \in HP, s \in S
\end{aligned}
$$

Additional auxiliary binary variables are used to simplify the formulation:

$$y^{a}_{i,s,e}=\begin{cases}1 & \text{if stream } i \text{ uses a compressor on shaft unit } e \text{ in stage } s\\ 0 & \text{otherwise}\end{cases} \quad i\in LP, s\in S, e\in E$$

$$y^{a}_{j,s,e}=\begin{cases}1 & \text{if stream } j \text{ uses a turbine on shaft unit } e \text{ in stage } s\\ 0 & \text{otherwise}\end{cases} \quad j\in HP, s\in S, e\in E$$

The following logical relationships are used for ensuring feasible solutions by reducing the search space.

$$1-y_{i,s,e,k}+y^{a}_{i,s,e}\geq 1 \quad i\in LP, s\in S, e\in E, k\in K \tag{A.1}$$

$$1-y^{a}_{i,s,e}+\sum_{k=1}^{K}y_{i,s,e,k}\geq 1 \quad i\in LP, s\in S, e\in E \tag{A.2}$$

$$1-y_{j,s,e,k}+y^{a}_{j,s,e}\geq 1 \quad j\in HP, s\in S, e\in E, k\in K \tag{A.3}$$

$$1-y^{a}_{j,s,e}+\sum_{k=1}^{K}y_{j,s,e,k}\geq 1 \quad j\in HP, s\in S, e\in E \tag{A.4}$$

In each compression and expansion stage should be placed a single-stage SSTC compressor/turbine (maximum three units disposed in parallel), and/or a stand-alone compressor/turbine, or bypass. Thus, the following binary variables are used to allow the bypass selection in each stage of the network:

$$y^{B}_{i,s}=\begin{cases}1 \text{ if stream } i \text{ bypasses stage } s\\ 0 \text{ otherwise}\end{cases} \quad i\in LP, s\in S$$

$$y^{B}_{j,s}=\begin{cases}1 \text{ if stream } j \text{ bypasses stage } s\\ 0 \text{ otherwise}\end{cases} \quad j\in HP, s\in S$$

The following logical relationships are needed to ensure the choice between stand-alone equipment and bypass.

$$y_{i,s}^{B} + y_{i,s}^{U} \le 1 \quad i \in LP,\ s \in S \tag{A.5}$$

$$1 - y_{i,s}^{B} + 1 - y_{i,s,e}^{a} \ge 1 \quad i \in LP,\ s \in S,\ e \in E \tag{A.6}$$

$$y_{j,s}^{B} + y_{j,s}^{U} + y_{j,s}^{V} \le 1 \quad j \in HP, s \in S \tag{A.7}$$

$$1 - y_{j,s}^{B} + 1 - y_{j,s,e}^{a} \ge 1 \quad j \in HP, s \in S, e \in E \tag{A.8}$$

Clearly, if there is bypass in a compression/expansion stage, it should occur in all succeeding stages (for ensuring that the bypass only occurs in the case that the stream target condition is reached).

$$1 - y_{i,s}^{B} + y_{i,s+1}^{B} \ge 1 \quad i \in LP, s \in S \tag{A.9}$$

$$1 - y_{j,s}^{B} + y_{j,s+1}^{B} \ge 1 \quad j \in HP, s \in S \tag{A.10}$$

In the case that there is *k* (max. 3 units) compressors allocated in parallel in a stage *s*, the next relationships are used to ensure the selection of split *k*–1 before the choice of split *k*.

$$1 - y_{i,s,e,k} + y_{i,s,e,k-1} \ge 1 \quad i \in LP, s \in S, e \in E, k \in K \tag{A.11}$$

$$1 - y_{j,s,e,k} + y_{j,s,e,k-1} \ge 1 \quad j \in HP, s \in S, e \in E, k \in K \tag{A.12}$$

Multiples SSTC units can be used in the network. Therefore, the following logical relationships are used to avoid the selection of the same axis twice.

$$1 - y_{i,s,e}^{a} + \sum_{i=1}^{LP}\sum_{s=1}^{S} y_{i,s,e-1}^{a} + \sum_{j=1}^{HP}\sum_{s=1}^{S} y_{j,s,e-1}^{a} \ge 1 \quad 1 \le i \le LP, s \in S, e \in E \tag{A.13}$$

$$1 - y^{a}_{j,s,e} + \sum_{i=1}^{LP}\sum_{s=1}^{S} y^{a}_{i,s,e-1} + \sum_{j=1}^{HP}\sum_{s=1}^{S} y^{a}_{j,s,e-1} \geq 1 \quad 1 \leq j \leq HP, s \in S, e \in E \tag{A.14}$$

Lastly, each compression and expansion stage in the superstructure should be selected only one time.

$$y^{B}_{i,s} + y^{U}_{i,s} + \sum_{e=1}^{E} y^{a}_{i,s,e} = 1 \quad i \in LP, s \in S \tag{A.15}$$

$$y^{B}_{j,s} + y^{V}_{j,s} + y^{U}_{j,s} + \sum_{e=1}^{E} y^{a}_{j,s,e} = 1 \quad j \in HP, s \in S \tag{A.16}$$

A.3 Compression and expansion stages

Pressure assignment. Assignment of streams pressure at the WEN entry and exit are given by **Eq. (A.17) – Eq. (A.20)**.

$$P_{IN\,i} = Pin_{i,1} \quad i \in LP, s = 1 \tag{A.17}$$

$$Pout_{i,S} = P_{OUT\,i} \quad i \in LP, s = S \tag{A.18}$$

$$P_{IN\,j} = Pin_{j,1} \quad j \in HP, s = 1 \tag{A.19}$$

$$Pout_{j,S} = P_{OUT\,j} \quad j \in HP, s = S \tag{A.20}$$

In which, streams pressures are limited by: $MIN\left[P_{IN}, P_{OUT}\right] \leq P \leq MAX\left[P_{IN}, P_{OUT}\right]$.

Mass balances. Mass balances at mixing points of the superstructure are given by the following equations.

$$F_i = Fu_{i,s} + Fb_{i,s} + \sum_{e=1}^{E}\sum_{k=1}^{K} Fe_{i,s,e,k} \quad i \in LP, s \in S \tag{A.21}$$

$$F_j = Fv_{j,s} + Fu_{j,s} + Fb_{j,s} + \sum_{e=1}^{E}\sum_{k=1}^{K} Fe_{j,s,e,k} \quad j \in HP, s \in S \tag{A.22}$$

Energy balances. Energy balances at mixing points are required due to the possibility of streams splitting in each stage.

$$F_j \cdot Tout_{j,s} = \begin{bmatrix} Fb_{j,s} \cdot Tin_{j,s} + Fv_{j,s} \cdot Tval_{j,s} + \\ \left(Fu_{j,s} + \sum_{e=1}^{E}\sum_{k=1}^{K} Fe_{j,s,e,k} \right) \cdot Tturb_{j,s} \end{bmatrix} \quad j \in HP, s \in S \tag{A.23}$$

Note that streams temperatures are limited by the constraints: $T^{LO} \leq T \leq T^{UP}$.

Pressure and temperature feasibilities. Streams pressure and temperature should monotonically increase in compression stages, and decrease in expansion ones:

$$Pout_{i,s} \geq Pin_{i,s} \quad i \in LP, s \in S \tag{A.24}$$

$$Tout_{i,s} \geq Tin_{i,s} \quad i \in LP, s \in S \tag{A.25}$$

$$Pout_{j,s} \leq Pin_{j,s} \quad j \in HP, s \in S \tag{A.26}$$

$$Tout_{j,s} \leq Tin_{j,s} \quad j \in HP, s \in S \tag{A.27}$$

Compression and expansion work. Compression work required by utility and SSTC units is, respectively, given by **Eq. (A.28)** and **Eq. (A.29)**.

$$Wu_{i,s} = Fu_{i,s} \cdot Cp_i \left(Tout_{i,s} - Tin_{i,s} \right) \quad i \in LP, s \in S \tag{A.28}$$

$$We_{i,s,e,k} = Fe_{i,s,e,k} \cdot Cp_i \left(Tout_{i,s} - Tin_{i,s} \right) \quad i \in LP, s \in S, e \in E, k \in K \tag{A.29}$$

Similar equations are used to estimate the energy generated by utility and SSTC turbines:

$$Wu_{j,s} = Fu_{j,s} \cdot Cp_j \left(Tin_{j,s} - Tturb_{j,s} \right) \quad j \in HP, s \in S \tag{A.30}$$

$$We_{j,s,e,k} = Fe_{j,s,e,k} \cdot Cp_j \left(Tin_{j,s} - Tturb_{j,s} \right) \quad j \in HP, s \in S, e \in E, k \in K \tag{A.31}$$

In which,

$$Tout_{i,s} = Tin_{i,s} \left[1 + \eta_i \left(Pout_{i,s} / Pin_{i,s} \right)^{(\gamma - 1/\gamma) - 1} \right] \quad i \in LP, s \in S \tag{A.32}$$

$$Tturb_{j,s} = Tin_{j,s} \left[1 + \eta_j \left(Pout_{j,s} / Pin_{j,s} \right)^{(\gamma - 1/\gamma) - 1} \right] \quad j \in HP, s \in S \tag{A.33}$$

In each WEN stage, the outlet pressure is restricted by a maximum compression ratio as follows.

$$CR_{\max} \geq \frac{Pout_{i,s}}{Pin_{i,s}} \quad i \in LP, s \in S \tag{A.34}$$

Expansion via valves is modeled as isenthalpic processes as given by **Eq. (A.35)**.

$$Tval_{j,s} = Tin_{j,s} + \mu_j \left(Pout_{j,s} - Pin_{j,s} \right) \quad j \in HP, s \in S \tag{A.35}$$

Bypass in a WEN stage. The following disjunction and big-M reformulation are used to allow for the bypass existence.

$$\begin{bmatrix} y^B_{i,s} \\ Tout_{i,s} = Tin_{i,s} \\ Pout_{i,s} = Pin_{i,s} \end{bmatrix} \veebar \begin{bmatrix} \neg y^B_{i,s} \\ Tout_{i,s} = Tin_{i,s} \left[1 + \eta_i \left(Pout_{i,s} \big/ Pin_{i,s} \right)^{(\gamma-1/\gamma)-1} \right] \end{bmatrix}$$

$$Tin_{i,s} - Tout_{i,s} \le M_{1i,s} \left(1 - y^B_{i,s} \right) \tag{A.36}$$

$$Tin_{i,s} - Tout_{i,s} \ge -M_{1i,s} \left(1 - y^B_{i,s} \right) \tag{A.37}$$

$$Pin_{i,s} - Pout_{i,s} \le M_{2i,s} \left(1 - y^B_{i,s} \right) \tag{A.38}$$

$$Pin_{i,s} - Pout_{i,s} \ge -M_{2i,s} \left(1 - y^B_{i,s} \right) \tag{A.39}$$

In which, $M_{1i,s} = Tin^{UP}_{i,s} - Tout^{LO}_{i,s}$ and $M_{2i,s} = Pin^{UP}_{i,s} - Pout^{LO}_{i,s}$.

If the stream does not bypass a stage, its flowrate through the bypass should be equal to zero. This is ensured by the following convex hull formulation:

$$Fb_{i,s} \le Fb^{UP}_{i,s} \cdot y^B_{i,s} \quad i \in LP, s \in S \tag{A.40}$$

$$Fb_{j,s} \le Fb^{UP}_{j,s} \cdot y^B_{j,s} \quad j \in HP, s \in S \tag{A.41}$$

The same should occur if valves or stand-alone equipment do not exist in a stage:

$$Fv_{j,s} \leq Fv_{j,s}^{UP} \cdot y_{j,s}^{V} \quad j \in HP, s \in S \tag{A.42}$$

$$Fu_{i,s} \leq Fu_{i,s}^{UP} \cdot y_{i,s}^{U} \quad i \in LP, s \in S \tag{A.43}$$

$$Wu_{i,s} \leq Wu_{i,s}^{UP} \cdot y_{i,s}^{U} \quad i \in LP, s \in S \tag{A.44}$$

$$Fu_{j,s} \leq Fu_{j,s}^{UP} \cdot y_{j,s}^{U} \quad j \in HP, s \in S \tag{A.45}$$

$$Wu_{j,s} \leq Wu_{j,s}^{UP} \cdot y_{j,s}^{U} \quad j \in HP, s \in S \tag{A.46}$$

A.4 Global energy balance in each SSTC axis

The global energy balance in the SSTC axis unit is given by the following equation.

$$Wg_e + \sum_{i=1}^{LP} \sum_{s=1}^{S} \sum_{k=1}^{K} We_{i,s,e,k} = Wm_e + \sum_{j=1}^{HP} \sum_{s=1}^{S} \sum_{k=1}^{K} We_{j,s,e,k} \quad e \in E \tag{A.47}$$

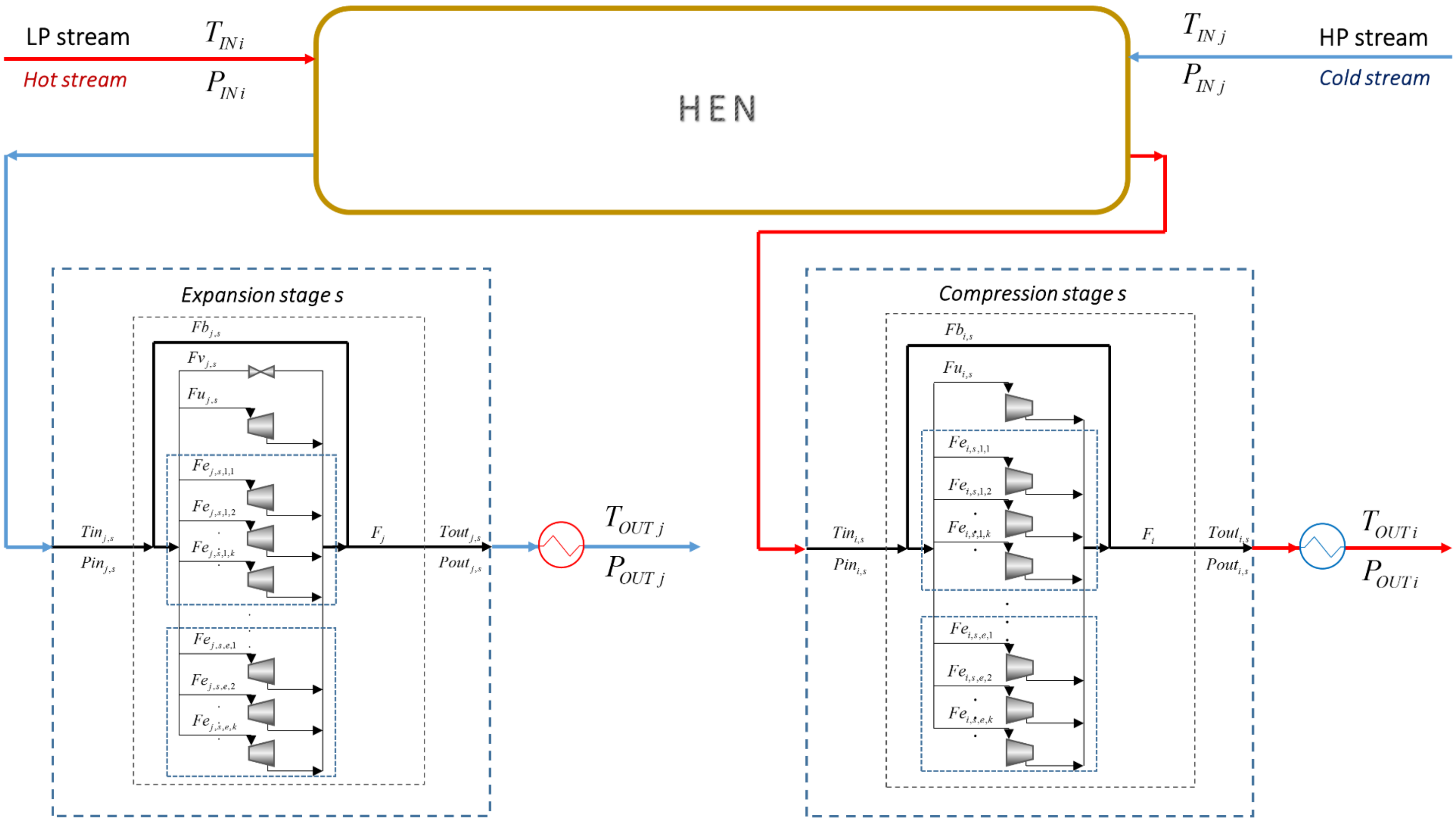

Fig. 1. Multi-stage superstructure and main decision variables considered for the multi-objective WHEN synthesis

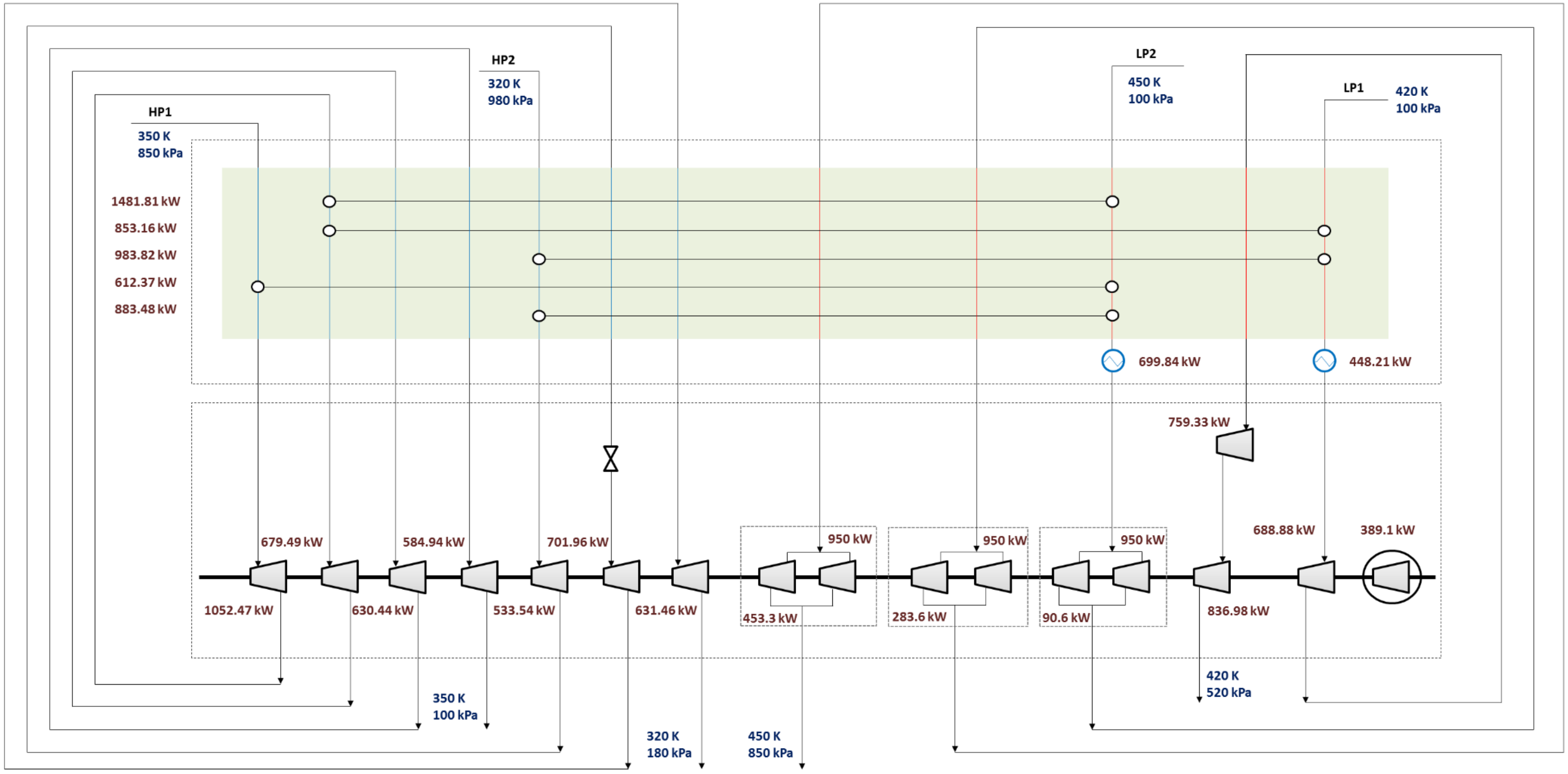

Fig. 2. Optimal WHEN configuration with minimum total environmental impact.

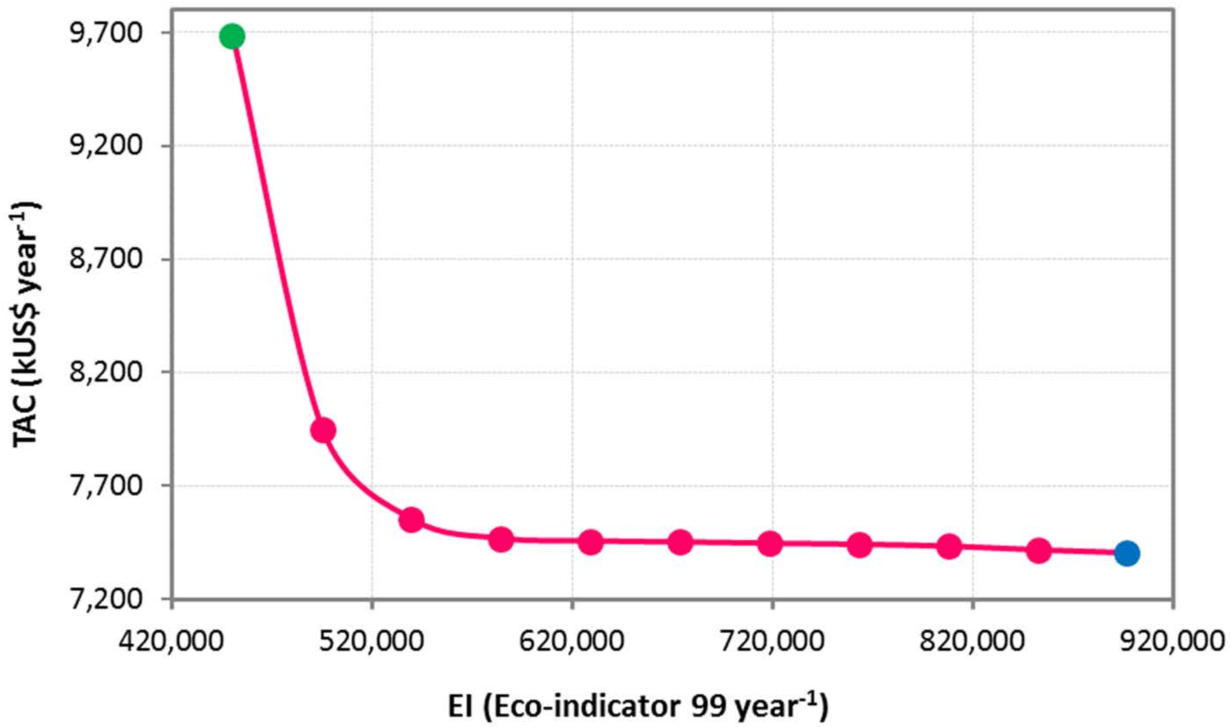

Fig. 3. Pareto curve of optimal alternative trade-off solutions for the case study.

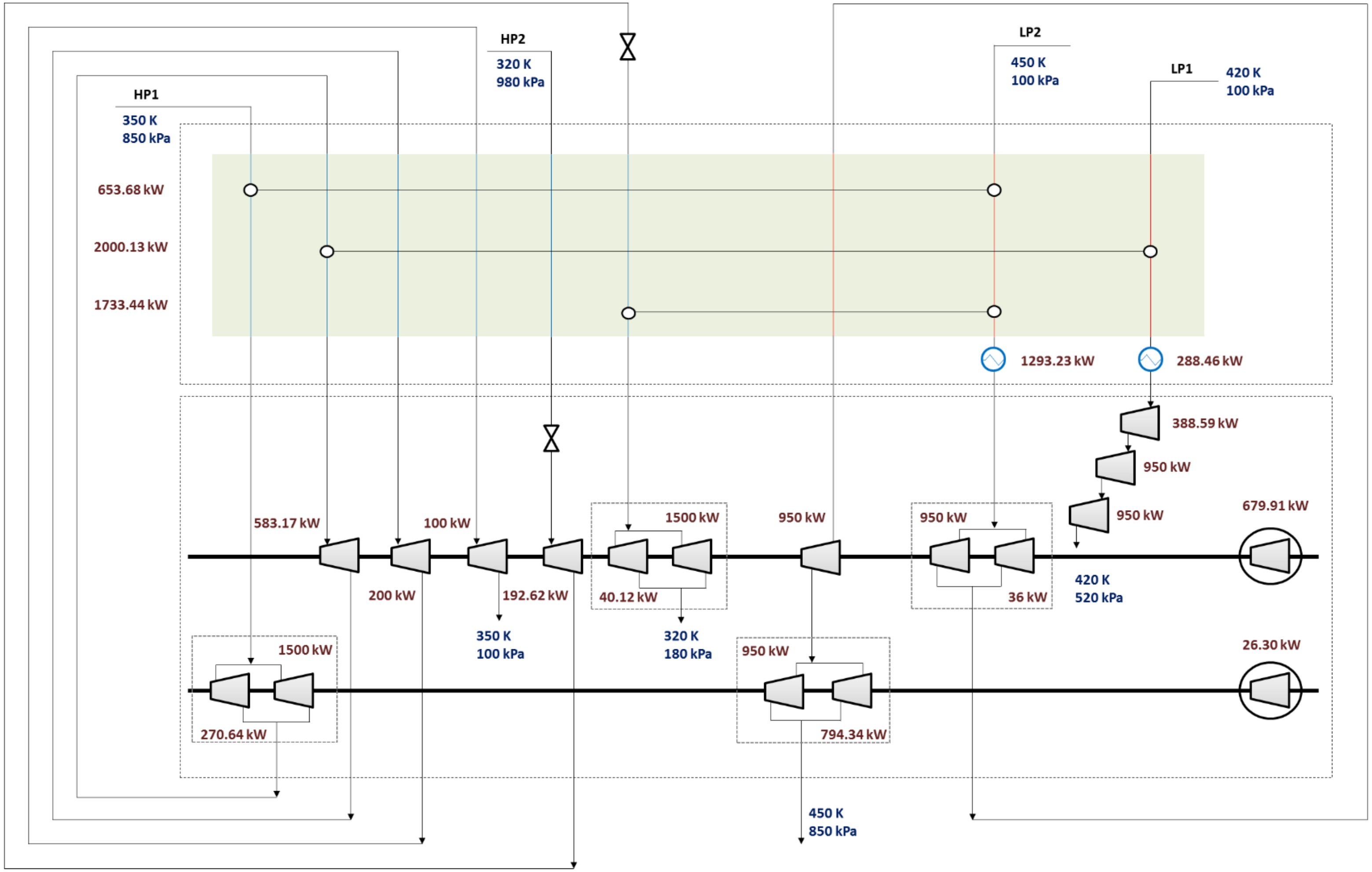

Fig. 4. Optimal WHEN configuration with minimum total annualized cost.

Table 1

Stream data, and environmental and cost parameters for the case study.

Stream	F (kg/s)	Cp (kJ/kg K)	T_{in} (K)	T_{out} (K)	P_{in} (kPa)	P_{out} (kPa)
HP1	15	1.432	350	350	850	100
HP2	18	0.982	320	320	980	180
LP1	15	1.432	420	420	100	520
LP2	18	1.432	450	450	100	850
Environmental data						
				Eco-indicator 99 (kW/h)*		
Steam				2,29E-02		
Cooling water				7,45E-05		
Electricity				4,90E-02		
Cost data (US$/year kW)						
Electricity cost (c_{elec})				850.5		
Electricity sale (c_{elec_sale})				750.0		
Heating service (c_{steam})				418.8		
Cooling service ($c_{cooling\_water}$)				100.0		

* *Ecoinvent default, LCIA, Eco99 (H/A), Europe/Es* [27].

Table 2

Optimal extreme solutions obtained in the case study.

Pareto extreme solutions	Total compression work (kW)	Total expansion work (kW)	Total heat transfer area (m^2)	Cooling services consumption (US$/year kW)	Electricity consumption (US$/year kW)	Capital cost (US$/year kW)	TAC (US$/year kW)	EI (1/year)
EI minimization	5,964	4,814	14,785	115	977	8,592	9,684	450,476
TAC minimization	5,968	4,387	3,180	158	1,417	5,829	7,404	897,317